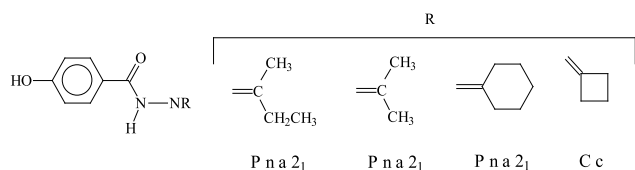


ionic chromophores, or the lowering of the rod-like symmetric shape of the molecule by introducing lateral substituents. Other approaches are based on crystal engineering strategies exploiting directional intermolecular interactions (e.g. H-bonding, halogen bonding), or supramolecular approaches as inclusion compounds and co-crystals [1].

However, all these approaches are highly empirical and fundamentally trial-and-error based. To get a polar crystal is still a challenging task.

Here, we report some preliminary results on the discovery of a class of nonchiral compounds forming polar crystal structures, with favourable orientation of the molecule with respect to the polar axis. Chemical diagrams of the compounds prepared up to now are given in the Scheme below, together with their space groups.

The angle between the polar axis and the long molecular axis joining phenolic oxygen to imino carbon is, respectively, 60°, 41°, 60° and 28° in the four compounds of the Scheme. The functionality resulting from the polar order of the first compound in the scheme has been confirmed by the powder second harmonic generation measurements by the method of Kurtz and Perry, where the efficiency is 120 % that of urea standard at the non-resonant fundamental wavelength of 1907 nm.



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Keywords: polar crystals, second harmonic generation, H-bonding synthons.

MS24.P09

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New coordination polymers with embedded molecular recognition functionality

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The use of molecular hosts as tectons for the self-assembly of coordination polymers promises crystalline materials with embedded molecular recognition sites, as well as the more common lattice-type guest sites [1], [2], [3], [4], [5]. We have developed a range of host molecules based on the cyclotrimeratrylene (CTV) framework with additional metal-binding groups at their upper rims.

Tripodal CTV-analogues have a distinctive open pyramidal shape which creates the specific guest-binding site. The rigid “corner-piece” shape also means that coordination polymers resulting from these ligands may have unusual structural and topological aspects to them. For example, 2D networks of linked metallo-cages; [1] rare (3,4)-connected network topologies such as (4².6²)(4.6²)₂; and highly complex and unprecedented 3D topologies [2].

As these tectons are molecular hosts, host-guest interactions may play an important role in both the assembly of the coordination polymers and in their potential applications. Host-guest associations may be structure-directing, and generally, binding large guests in the molecular cavity of the ligand promotes formation of a coordination

polymer instead of a discrete species [3], [4]. For example, binding of a large *o*-carborane guests dictates whether a discrete [Cd₃(OAc)₆L] complex or 2D 4.8² coordination polymer is formed when L = tris(4-pyridyl)aminocyclotrimeratrylene [3] Self-inclusion motifs also play an important role. Crystalline clathrates of CTV-analogues are known to form a hand-shake dimer where an upper-rim R group of one host is the guest for another host and vice versa, and the same motif is found within coordination chains [5]. Host-guest interactions may also result in associations between networks, including within polycatenation motifs.

Here, different coordination polymers from ligands with N-donor, carboxylate, N-oxide or allyl metal-binding groups will be presented, and the importance of host-guest interactions of these ligands in terms of coordination polymer construction and functionality highlighted.



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Keywords: supramolecular, crystal engineering, coordination polymers

MS24.P10

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Kinetic assembly of porous coordination networks and *ab initio* powder structure determination

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The chemistry of porous coordination networks has undergone explosive growth in the last decade because of fascinating features. Porous coordination networks can be used for gas sorption/separation/storage, molecular recognition, drug delivery, catalysis, and so on. Especially porous materials have been paid much attention as potential hydrogen storage materials for fuel cells. Thanks to the high flexibility in design, a number of porous coordination networks were prepared and were analyzed by single crystal X-ray crystallography. Here we would like to report new aspects in porous coordination network chemistry. A pore of porous materials can be used as crystalline molecular flask in order to not only make a reaction but also directly observe the reaction by X-rays [1-5]. In this talk, especially we will focus on selective kinetic assembly of porous coordination networks, the usage, and the *ab initio* powder structure determination [6-10]. The kinetic study of porous coordination networks compared with zeolite is a totally unexplored field, because of difficulties in powder structure determination. We succeeded in solving powder crystal structures having unit cells larger than 15000 Å³.

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